Relation between classical and quantum particle systems

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An exact correspondence is established between a N-body classical interacting system and a $(N-1)$-body quantum system with respect to the partition function. The resulting Hermitian quantum potential is a $(N-1)$-body one. Inversely the Kelbg potential is reproduced which describes quantum systems at a quasiclassical level. The correspondence found between classical and quantum systems allows also to approximate dense classical many-body systems by lower order quantum perturbation theory, replacing Planck's constant properly by temperature and density dependent expressions. As an example, the dynamical behavior of a one-component plasma is well reproduced concerning the formation of correlation energy after a disturbance, utilizing solely the analytical quantum-Born result for dense degenerated Fermi systems. As a practical guide, the quantum-Bruckner parameter r_s has been replaced by the classical plasma parameter Γ as $r_s \approx 0.3\Gamma^{3/2}$.

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Several hints in the recent literature conjecture that there exists a correspondence between quantum systems and higher dimensional classical systems. The authors of Ref. [1] argue that a higher dimensional classical non-Abelian gauge theory leads to a lower dimensional quantum field theory in the sense of chaotic quantization. The correspondence appears by equating the temperature characterizing chaotization of the higher dimensional system with $\hbar$ of the lower dimensional system by

$$\hbar = aT. \tag{1}$$

Recalling the imaginary time evolution as a method to calculate correlated systems in equilibrium such correspondence seems suggestible. We will find a similar relation as a best fit of quantum-Born calculations to dense interacting classical systems.

In condensed matter physics it is a commonly used trick to map a two-dimensional classical spin system onto a one-dimensional quantum system [2]. This suggests that there might exist a general relation between quantum and higher dimensional classical systems. We will show that a classical many body system can be equally described by a quantum system with one particle less in the system but with the price of complicated nonlocal potential. This can be considered analogously to the Bohm̈ interpretation of quantum mechanics [3] where the Schrdinger equation is rewritten in a Hamilton-Jacobi equation but with a nonlocal quantum potential.

Another hint towards a correspondence between classical and quantum systems was found recently in Ref. [4] where it was achieved to define a Lyapunov exponent in quantum mechanics by employing the marginal distribution which is a representation of Wigner function in a higher dimensional space. Since the Lyapunov exponent is essentially a concept borrowed from classical physics, this finding points also in the direction that there exists a correspondence between quantum systems and higher dimensional classical systems.

On the opposite side there are systematic derivations of constructing effective classical potentials such that the many body quantum system is described by the classical system. An example is the Kelbg potential for Coulomb systems [5–8],

$$V_{12}^{\mathrm{Kelbg}}(r) = \frac{e_1 e_2}{r}\left[1 - \mathrm{e}^{-r^2/l^2} + \sqrt{\pi}\,\frac{r}{l}\,\mathrm{erfc}\left(\frac{r}{l}\right)\right], \tag{2}$$

with $l^2 = \hbar^2/2\mu T$ and $1/\mu = 1/m_1 + 1/m_2$ describing the two-particle quantum Slater sum correctly by a classical system. Improvements and systematic applications can be found in Refs. [9–11].

Here in this paper we show that a classical N-particle system can be mapped exactly on a quantum $(N-1)$-particle system with respect to the partition function. Though the resulting effective $(N-1)$-body quantum potential is highly complex, it can lead to practical applications for approximating strongly correlated classical systems. In the thermodynamical limit it means that the dense classical system can be described alternatively by a quantum system with properly chosen potential.

This finding suggests that the quantum calculation in lowest order perturbation might be suitable to derive good approximations for the dense classical system. This is also motivated by an intuitive picture. Assume that we have a dense interacting classical plasma system. Then the correlations will considerably restrict the possible phase space for traveling of one particle like in dense Fermi systems at low temperatures where the Pauli exclusion principle restricts the phase space for scattering. Therefore we might be able to describe a dense interacting classical system by a perturbative quantum calculation when we properly replace $\hbar$ by density and temperature expressions. Indeed we will demonstrate in a one-component plasma system that even the time evolution and dynamics of a very strongly correlated classical system can be properly approximated by quantum-Born calculations.

Let us now derive the equivalence between classical and quantum systems by rewriting the classical N-particle configuration integral

$$Q_N(\beta) = \int dx_1 \cdots dx_N \prod_{i<j}^{N} (1 + f_{ij}), \tag{3}$$

where $f_{ij}=\exp[-\beta u_{ij}(x_i-x_j)]-1$ are the Meyer graphs with the interaction potential $u_{ij}(x_i-x_j)$ of the classical particles and the inverse temperature β. The subscripts in u_{ij} denote the coupling constants like charges, etc. Consider now the modified configuration integral

$$\begin{aligned}\tilde{Q}_N(\beta)&=Q_N(2\beta)\\&=\int dx_1\cdots dx_N dx_1'\cdots dx_{N-1}'\delta(x_1-x_1')\cdots\delta(x_{N-1}-x_{N-1}')\\&\quad\times(1+f_{12})(1+f_{13})(1+f_{14})\cdots(1+f_{1N})\\&\quad\times(1+f_{21'})(1+f_{23})(1+f_{24})\cdots(1+f_{2N})\cdots\\&\quad\times(1+f_{N1'})(1+f_{N2'})(1+f_{N3'})\cdots(1+f_{NN-1'}),\end{aligned}\tag{4}$$

such that a quadratic schema in the indices appears. Now we assume a complete set of $(N-1)$ particle wave functions $\Psi_{n_{N-1}}$ such that

$$\begin{aligned}&\delta(x_1-x_1')\cdots\delta(x_{N-1}-x_{N-1}')\\&\quad=\sum_{i_1\cdots i_{N-1}}\Psi^*_{i_1\cdots i_{N-1}}(x_1'\cdots x_{N-1}')\Psi_{i_1\cdots i_{N-1}}(x_1\cdots x_{N-1}),\end{aligned}\tag{5}$$

with "quantum numbers" $\{i\}$ characterizing the state. Further we propose the following eigenvalue problem defining the wave function:

$$\begin{aligned}\int dx_1\prod_{j=2}^{N}(1+f_{1j})\Psi_{i_1\cdots i_{N-1}}(x_1\cdots x_{N-1})\\=Ve^{-\varepsilon_{\{i\}}}\Psi_{i_2\cdots i_{N-1}i_1}(x_2\cdots x_N),\end{aligned}\tag{6}$$

with the system volume V. This allows us to calculate the configurational integral (4) exactly by successively integrating $x_1\cdots x_N$, with the result

$$\tilde{Q}_N(\beta)=V^N\sum_{i_1\cdots i_{N-1}}e^{-N\varepsilon_{\{i\}}}.\tag{7}$$

This already establishes the proof that we can map a classical N-body system on a $(N-1)$-body quantum system since Eq. (6) is the eigenvalue problem of a $(N-1)$-body Schrödinger equation. To see this we can consider a wave function ξ built from the Fourier transform of Ψ,

$$\begin{aligned}\xi(p_1\cdots p_{N-1},t)=\exp\left[-\frac{i}{\hbar}\left(\sum_{i=1}^{N-1}\frac{p_i^2}{2m_i}-E_{N-1}\right)t\right]\\\times\tilde{\Psi}_{i_1\cdots i_{N-1}}(p_1\cdots p_{N-1}),\end{aligned}\tag{8}$$

which obeys the $(N-1)$-particle Schrödinger equation

$$\left(i\hbar\frac{\partial}{\partial t}-\sum_{i}^{N-1}\frac{p_i^2}{2m_i}-\tilde{U}\right)\xi(p_1\cdots p_{N-1},t)=0,\tag{9}$$

with $E_{N-1}=\Omega Ve^{-\varepsilon_{\{i\}}}$ and we rewrote the left hand side of Eq. (6) as quantum potential

$$\begin{aligned}&\langle x_1 i_1\cdots x_{N-1}i_{N-1}|U|x_1'i_1'\cdots x_{N-1}'i_{N-1}'\rangle\\&\quad=e^{\beta[u_{12}(x_1'-x_1)+\cdots+u_{1N}(x_1'-x_{N-1})]}\Omega\,\delta(x_1-x_2')\\&\qquad\times\cdots\delta(x_{N-2}-x_{N-1}')\,\delta_{i_1',i_1}\cdots\delta_{i_{N-1}',i_{N-1}}.\end{aligned}\tag{10}$$

Here Ω is an arbitrary energy density setting up the energy scale. The resulting Hermitian quantum potential (10) is a $(N-1)$-body nonlocal potential with respect to the coordinates but depends on N strength function parameter (e.g., charges). Therefore we have cast a classical N-body problem into a nonlocal quantum $(N-1)$-body problem.

While the above correspondence holds for any particle number and might be useful to find solvable models for classical three-body problems, we will consider many-body systems in the following. First let us invert the problem and search for an effective classical potential approximating quantum systems. This should lead us to the known Kelbg-potential (2). For this purpose we assume a quantum system described in lowest approximation by a Slater determinant or a complete factorization of the many-body wave function into a single wave function $\Psi_{i_1\cdots i_N}(x_1\cdots x_N)=\phi_{i_1}\cdots\phi_{i_N}$. For simplicity, we neglect the exchange correlations in the following. The corresponding eigenvalue equation for ϕ itself one can obtain from Eqs. (6) or (9) by multiplying with $\Psi^*_{i_2\cdots i_{N-1}}(x_2\cdots x_{N-1})$ and integrating over $x_2\cdots x_{N-1}$. To see the generic structure more clearly we better calculate the correlation energy by multiplying Eq. (6) or Eq. (9) by $\Psi^*_{i_2\cdots i_{N-1}i_1}(x_2\cdots x_N)$ and integrating over $x_2\cdots x_N$. This provides also the eigenvalue $\epsilon_{\{i\}}$ and leads us easily to the approximations for the partition function (3). To demonstrate this we choose the lowest order approximation taking identical plane waves for ϕ. Then the pressure can be obtained from the partition function Q_N via (7)

$$P=T\frac{\partial}{\partial V}\ln Q_N=T\left(\frac{N}{V}-\frac{N(N-2)}{V^2}\int dr(e^{-\beta u(r)/2}-1)\right),\tag{11}$$

where V is the volume of the system. We recognize the standard second virial coefficient for small potentials while for higher order potential the factor 1/2 appears in the exponent instead as a prefactor indicating a different partial summation of diagrams due to the different schema behind Eqs. (7) and (9).

To go beyond the plane wave approximation we multiply Eq. (6) by $\Psi^*_{i_2\cdots i_{N-1}i_1}(x_2\cdots x_N)$ and the kinetic part of the statistical operator before integrating over $x_2\cdots x_N$. This means we create an integral over the $N-1$ particle density operator and the potential (10) which together represents the correlation energy. This expression is a successive convolution between the cluster graphs f_{ij} and the relative two-particle correlation function $\rho_{i_1i_2}(x_1-x_2)$. The resulting correlation energy density reads

$$\frac{U}{V}=\sum_{\{i\}}\int\frac{dy_1\cdots dy_{N-1}}{V^{N-1}}$$
$$\times\rho_{i_1i_2}(y_1)\rho_{i_2i_3}(y_2)\cdots\rho_{i_{N-1}i_1}(y_{N-1})[1-f_{12}(y_1)]$$
$$\times[1-f_{13}(y_1+y_2)]\cdots[1-f_{1N}(y_1+\cdots+y_{N-1})]$$
$$\approx\sum_{\{i\}}\int\frac{dy_1\cdots dy_{N-1}}{V^{N-1}}\rho_{i_1i_2}(y_1)\cdots\rho_{i_{N-1}i_1}(y_{N-1})$$
$$\times u_{12}(y_1)u_{13}(y_1+y_2)\cdots u_{1N}(y_1+\cdots+y_{N-1})+\cdots \tag{12}$$

in dimensionless units where all other cluster expansion terms lead either to lower mean field or disconnected terms. While these terms can also be calculated we restrict to the highest order convolutions in the correlation energy (12) which indeed have the structure of a correlation energy $U/V=\Sigma_{i_1i_2}\int(dx/V)\rho_{i_1i_2}(x)V_{12}^{\mathrm{eff}}$ with the classical effective potentials

$$V_2^{\mathrm{eff}}(r)\propto\sum_3\int\frac{dx_1}{V}\rho_{12}(x_1)u_{12}(x_1)u_{23}(x_1+r), \tag{13}$$

$$V_3^{\mathrm{eff}}(r)\propto\sum_{34}\int\frac{dx_1dx_2}{V^2}\rho_{12}(x_1)u_{12}(x_1)u_{13}(x_1+x_2)$$
$$\times\rho_{23}(x_2)u_{34}(x_1+x_2+r), \tag{14}$$

according to the two particle, three particle, etc., approximation read off from Eq. (12). In equilibrium the nondegenerate correlation function reads $[l^2=\hbar^2/\mu T=\lambda^2/2\pi]$

$$\rho_{i_1i_2}(x_1-x_2)=\int\frac{dp}{(2\pi\hbar)^3}e^{ipr/\hbar}\lambda^3\exp\left(-\beta\frac{p^2}{2\mu}\right)=e^{-r^2/l^2}. \tag{15}$$

Using the Coulomb potential $u\propto 1/r$ we obtain from the two-particle approximation (13) just the Kelbg potential (2). The three-particle approximation (14) can be calculated as well and reads $[x=r/l]$

$$V_3^{\mathrm{eff}}\sim\frac{1}{x}\left[\mathrm{erf}^2\left(\frac{x}{\sqrt{2}}\right)+\frac{2^{3/2}x}{\sqrt{\pi}}\int_x^\infty\frac{dz}{z}\exp\left(-\frac{z^2}{2}\right)\mathrm{erf}\left(\frac{z}{\sqrt{2}}\right)\right]. \tag{16}$$

The third order potential is somewhat less bound than the Kelbg potential as can be seen in Fig. 1. With the schema (14) one can easily integrate higher order approximations as successive convolutions, but with respect to the small differences between Eqs. (2) and (16) in Fig. 1 one does not expect much change. Also, in principle the degenerate case could be calculated using Fermi-Dirac distributions in Eq. (15). But one should then consider also the neglected exchange correlations during factorization of Ψ as well. Let us summarize that the known effective classical potential describing a quantum system in binary approximation has been recovered by identifying the effective two-particle interaction within the correlation energy.

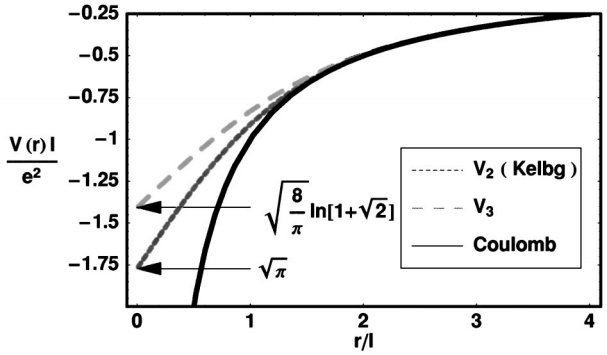

FIG. 1. The comparison of the Kelbg potential (2) and the third order potential (16) vs r/l.

We now want to proceed to a phenomenological level in that the above correspondence between quantum and classical systems motivates us to find good approximations even for the dynamics of classical many-body systems by employing quantum-Born approximations. This can be understood by the fact that the Kelbg potential deviates appreciably from the Coulomb one, only if the interparticle distance d is smaller than the thermal wavelength λ. In other words, for dense classical systems under such conditions we can think of it as a dilute quantum system replacing $\lambda\sim d$. To check this conjecture let us consider a one-component plasma which is characterized by two values. The classical coupling is described by the plasma parameter $\Gamma=e^2/dT$, as a ratio of the length where Coulomb energy becomes larger than kinetic energy, e^2/T, to the interparticle distance or Wigner size radius $d=(3/4\pi n)^{1/3}$. Ideal plasmas are found for $\Gamma\ll 1$ while around $\Gamma=1$ nonideal effects become important. A second parameter which controls the quantum features is the Bruckner parameter as the ratio of the Wigner size radius to the Bohr radius $a_B=\hbar^2/me^2$. Quantum effects will play a role if $r_s\leqslant 1$. We will consider the situation where the interaction of such a system is switched on at the initial time. Then the correlations are formed by the system which is seen in an increase of temperature accompanied by the buildup of negative correlation energy. This theoretical experiment has been investigated numerically by Ref. [12] for classical plasmas with different plasma parameter Γ.

In Refs. [13,14] we have calculated the formation of such correlations by using quantum kinetic equations in Born approximation. The time dependence of kinetic energy was found at short times to be

$$E_{\mathrm{corr}}=-\sum_{ab}\int\frac{dk\,dp\,dq}{(2\pi\hbar)^9}V_D^2\frac{1-\cos\left\{\frac{1}{\hbar}t\Delta_E\right\}}{\Delta_E}$$
$$\times f_a'f_b'(1-f_a)(1-f_b), \tag{17}$$

where f are the initial distributions and

$$\Delta_E=\frac{k^2}{2m_a}+\frac{p^2}{2m_b}-\frac{(k-q)^2}{2m_a}-\frac{(p+q)^2}{2m_b}.$$

The statical screened Coulomb interaction is $V_D(q) = 4\pi e^2\hbar^2/(q^2+\hbar^2\kappa^2)$. The inverse screening length is given by $\kappa^2 = 4\pi e^2 n/T$ for the high or by $\kappa^2 = 6\pi e^2 n/\epsilon_f$ for the low temperature limit in terms of the density n and the temperature T. For both the cases, dynamical as well as statical screening, it was possible to integrate analytically the time dependent correlation energy (17). This has allowed to describe the time dependence of simulations in the weak coupling limit $\Gamma<1$ appropriately [13]. For stronger coupling $\Gamma \geqslant 1$ the Born approximation fails since the exact correlation energy of simulation is lower than the first order (Born) result $\kappa e^2/2T = \sqrt{3/2}\Gamma^{3/2}$. Moreover, there appear typical oscillations, see Fig. 2.

Now we employ the ideas developed above and use the quantum-Born approximations in the strongly degenerated case to describe the classical strongly correlated system. For strongly degenerated plasmas the time dependence of correlation energy was possible to integrate as well with the result [14] expressed here in terms of plasma parameter Γ and quantum Bruckner parameter r_s as

$$\frac{E^T_{\rm corr}(t)-E^0_{\rm corr}(t)}{nT} = \frac{1}{(36\pi^4)^{1/6}}\frac{r_s^3}{\Gamma}\left(\frac{\sin y\tau}{y\tau}-1\right) \times\left[\frac{1}{b_l}\arctan\left(\frac{1}{b_l}\right)+\frac{1}{b_l^2+b_l^4}\right], \quad (18)$$

with $b_l = \hbar\kappa/2p_f = \sqrt{\Gamma}/(48\pi^2)^{1/6}$, $y\tau = 4\epsilon_f t/\hbar = (2)^{4/3}\pi^{5/3}3^{5/6}\tau/\sqrt{r_s}$ where the time is scaled in plasma periods $\tau = 2\pi t/\omega_p$. Now we fit this quantum result to the simulation using the Bruckner parameter as a free parameter. For the available simulations between $1\leqslant\Gamma\leqslant 10$ we obtain a best fit

$$r_s^{\rm fit} = c\sqrt{\frac{3}{8}}\Gamma^{3/2}, \quad c\approx 0.5. \quad (19)$$

The quality of this fit is illustrated in Fig. 2 which is throughout the range $1\leqslant\Gamma\leqslant 10$. This is quite astonishing since not only is the correct classical correlation energy [15] described but also the correct time dependence, i.e., dynamics. Let us try to understand what this phenomenological finding means.

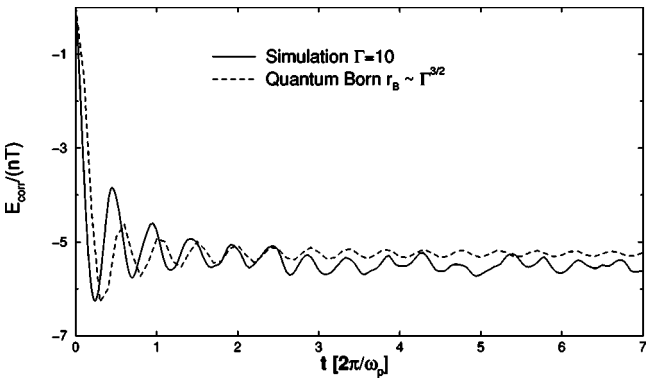

FIG. 2. The time evolution of a classical one-component plasma after sudden switching of interaction [12] compared to the quantum-Born result when the Bruckner parameter is replaced according to Eq. (19). The long time equilibrium value is remarkably well reproduced by the quantum-Born result (18).

Using the thermal de Broglie wavelength $\lambda^2 = \hbar^2/4mT$ we can rewrite Eq. (19) as $\lambda^2 \approx d/\kappa = d^2/(3\Gamma)^{1/2}$. In the considered range of $\Gamma = 1,\ldots,10$ we have $(3\Gamma)^{1/4} = 1,\ldots,2$ and the thermal wavelength λ is found to be nearly equal to the interparticle distance d as a best fit of the quantum-Born calculation to the dense classical system. This is exactly the distance where the Kelbg potential (13) or (2) starts to deviate from the Coulomb potential. In other words we confirm the conjecture that the dense classical system can be described by a dilute quantum system if in the latter the thermal wavelength is replaced by the interparticle distance. This condition (19) can also be rewritten into the result (1) of literature using the degenerated screening length.

We summarize that in equilibrium we have shown that there exists an exact relation between a N-body classical system and a $(N-1)$-body quantum system. This has allowed to recover the quantum Kelbg potential more easily. As a practical consequence I suggest to describe the dynamics of dense interacting classical many-body systems by the simpler perturbative quantum calculation in the degenerate limit, properly replacing $\hbar$ by typical classical parameters of the system.

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